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SCHOOL OF SCIENCES AND HEALTH PROFESSIONS
OLD DOMINION UNIVERSITY
NORFOLK, VIRGINIA

Technical Report PGSTR-AP76-21

(NASA-CP-146307) PARAMETERIZATION OF
GASEOUS CONSTITUENCIES CONCENTRATION
PROFILES IN THE PLANETARY BOUNDARY LAYER AS
REQUIRED IN SUPPORT OF AIRBORNE AND
SATELLITE BORNE (old Dominion Univ.

N76-19596
HC \$3.50
Unclassified
G3/45 18459

PARAMETERIZATION OF GASEOUS CONSTITUENCIES CONCENTRATION
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IN SUPPORT OF AIRBORNE AND SATELLITE BORNE SENSORS

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Prepared for the
National Aeronautics and Space Administration
Langley Research Center
Hampton, Virginia

Under

Grant NSG 1127

February 1, 1975 - January 31, 1976



March 1976

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1. BACKGROUND

The overall objective of this program is the development of capabilities for sensing air pollution constituents using satellite or airborne remote sensors. The thrust of this research is to focus on passive sensing of emissions in selected infrared bands. A number of general problem areas that must be addressed were definable from the outset. Two of the major problems are:

a. The constituent objectives of the sensor development are rarified trace elements in the atmosphere. Even with highly selective spectral bands, their total emitted energy from such small masses may be small compared to the spectral band components of near-black-body emission from the Earth or the contributions from the more dense substances like water vapor.

b. The vertically integrated radiance values measured by the sensor introduce an inherent ambiguity in the gaseous concentrations and temperatures at various layers in a highly vertical column of the atmosphere.

The signal-to-noise ratio problems suggested in (a) above appear to be reduced by a specially designed filtered sensor

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developed according to Langley Research Center (LaRC) specifications. This sensor was designed to measure CO concentrations and presumably reduces the relative magnitudes of the contributions from the Earth surface and water vapor by measuring the difference between a narrow infrared band radiance values of an unfiltered sensor and a value filtered through as a controllable amount of CO.

The initial phase of this research program was divided into two distinct parallel but mutually supporting phases. One has been concerned with the evaluation of the sensor in the pseudo-realistic environments and the second is the diagnosis of specific problems and development of techniques associated with application of the sensor in its conceptual "use" phase. Both phases of this effort have been conducted by Old Dominion University (ODU) personnel, but because of availability of facilities, it has been conducted in two physical locations; i.e., ODU and LaRC. The bulk of the evaluation effort, numerical integration of radiative transfer equations to reduce sensor data has been conducted at LaRC, while the bulk of the application diagnostic effort has been conducted at ODU. Both components were coordinated in the field experiments and are kept updated periodically by a schedule of informal technical exchange and planning briefings.

2. REVIEW OF RESULTS TO DATE

a. Sensor Evaluation Phase

(1) Ground truth analysis: In this critical area, a major problem became evident in the very early phases of the study; the definition of reliable ground truth needed to evaluate sensor data collected in field experiments. This proved to be a formidable problem that demanded a thorough examination of the present state of the science. Fortunately, significant progress has been achieved here. After considerable literature research, consultation with scientific peers on a national level, and extensive laboratory development effort, a technique has now been developed to do surface or ground truth measurements for CO and CH₄ to serve as cali-

bration points for the remote sensor data. The procedure developed is basically a gas chromatographic technique using a flame ionization detector. Cold traps serve to preconcentrate the trace gases of interest and measurements as low as 0.10 ppm are easily made with a noise equivalent concentration of 7 ppb.

The gas chromatograph is used here for point sampling and not continuous monitoring. Bottle samples, therefore, are taken as part of the ground truth both at the surface and at altitude when the remote sensor is flown. The bottles are then analyzed at a later date but as soon after the rest as possible. Difficulty with erratic data from bottle samples has led to a study of containerized gas sampling in general with special emphasis on statistical studies of the repeatability of our stainless steel bottles. Glass sample bottles have also been under study in an attempt to determine what type of container is best suited to ambient air sampling for trace gases.

During this reporting period, analysis were made on bottle samples and standard gases solely for the purpose of gathering statistics on the bottles used for the remote sensor ground truth program being conducted at LaRC. One summer field test of the remote sensor was conducted during the period requiring ground truth data and was reported in an earlier report.

The glass bottles which came equipped from the manufacturers with teflon stopcocks would not hold pressure. The stopcock fitting simply was not tight enough to hold 30 psi gauge, so the bottles were sent to the LaRC glass shop to be modified. One end was sealed off and the other end received a Glass-to-Kovar fitting on which a valve could be attached. The valve seals so that the bottle will hold 30 psi of sample gas.

Another repeatability study was done using the stainless steel bottles filled with ambient air. Air was sampled along the James River on Chesapeake Boulevard in 60 of the bottles. The repeatability at the ambient level for the stainless steel bottles did not appear to be as good as it was with the 1 ppm standard gas.

However, the 60 bottles were filled during a one-half hour period, and therefore some variation may be expected. In addition, several of the bottles which read high in the past read high in this study also. The results are not conclusive.

The same studies were conducted again, except that the glass bottles were used for comparison. The glass bottles were first filled with the 1 ppm standard gas. Analysis of these samples showed an excellent repeatability of approximately 1 percent for the 1 ppm standard gas. The CO repeatability looked very good even at the ambient air level in the glass bottles, about 10 percent from one bottle to the next. It was thought that an integrator might improve on this number since eyeball measurements of small peaks are difficult, so an integrator was purchased from Varian and arrived in mid-November. These tests in both the glass and stainless steel bottles with standard gases and ambient air were to be repeated once again using the integrator for data reduction instead of the hand method.

However, difficulty was encountered in getting the system to operate at peak sensitivity once it was shut off for any extended time period. Also, a contaminant appeared and then disappeared without explanation, causing some delay in repeating the tests. When the system was finally operational again, the studies were resumed on the glass bottles and the integrator began to fail intermittently.

The Varian repair person came, but was unable to locate the problem. As yet the problem remains unsolved. The integrator either does not integrate peaks or else it gives much too large an integration for a single peak. New circuit boards were ordered for the machine and hopefully it will perform as it should with the new boards. The bottle studies will then be resumed.

A 10-foot molecular sieve glass column was installed in the chromatograph in hopes of being able to raise the temperature of the oven to the point where the proportional controller would control the oven temperature. The stainless steel column was operated at approximately 60 °C, but heat leakage from the

detector housing is so great that the temperature was usually about 50° to 60 °C without the proportional controller working. The controller will serve to stabilize the oven temperature precisely regardless of the room temperature.

The remaining statistical repeatability studies will be conducted with or without a properly functioning integrator. Hopefully, the new circuit boards will improve the integrator's performance and enable it to be used in these tests.

A flight test of the remote sensor is scheduled for the first week in March and will require the taking of ground truth.

(2) Reduction of data through numerical integration of radiative transfer equations. In this subcategory, research has been performed in experimental and theoretical investigations of physical phenomena and processes in the Earth's atmosphere associated with the development of an experimental means of remotely measuring concentrations of gaseous constituents of the atmosphere via the application of the gas filter correlation (GFC) technique as described by Ludwig (ref. 1).

In May 1975 assistance was rendered in formalizing the June 1975 test flight which would evaluate the performance of the SR and T version of the gas filter correlation instrument over homogeneous and non-homogeneous background terrain in the Edenton, North Carolina and Albemarle Sound areas. For the actual flights, day and night, supporting and corroborating data in the form of collection of air samples, local air and water surface temperature measurements, and local observation of weather conditions was supplied by an ODU research vessel stationed on the Sound. In addition to these data, radiosonde information obtained from the Cape Hatteras station was used in computing a mathematical model of the local atmospheric conditions of the day and night flights. These models were used in conjunction with an atmospheric radiative transfer program, POLAYER III, to relate the GFC instrument measurements to the total vertical column density of trace atmospheric CO as described by Casas (ref. 2). Simultaneously, POLAYER III was used to investigate the theoretical sensitivity of measurement of a constituent gas by

the SR and T version of the GFC to uncertainties in atmospheric temperature profile. In August these investigations were terminated as a result of large errors in the inferred concentrations of CO for the reduced June flight data. The origin of these errors was investigated and determined to be the result of apparent errors in the integration interval methodology in the POLAYER III program. Assistance in altering the program to correct this problem was successful; however, the task was very difficult and time consuming due to the inflexibility of the POLAYER III program coding.

At this phase of development the lack of speedy turnaround time made it apparent that the present data reduction procedure had proven to very time- and cost-inefficient as shown by figure 1. The old procedure was analyzed and suggestions for new hardware and software requirements were implemented. A new digital data acquisition system, Pulse Code Modulation (PCM), resulted in a reduction of several weeks in the data reduction process. However, this improvement did not effectively reduce the total cost nor the time of the complementing steps of the old procedure. In late October the feasibility of developing a more efficient atmospheric radiative transfer program was investigated and was initiated in November. During November and December the integration of mathematical and physical concepts by ODU personnel with the programming optimization and development by personnel from the Vought Corporation resulted in the development of the mainline of the Simulated Monochromatic Atmospheric Radiative Transfer (SMART) program. Preliminary investigations found considerable reduction in cost and a higher degree of flexibility and efficiency in the data reduction procedure via the usage of the SMART program. Under the proposed data analysis procedure, illustrated in figure 2, the estimated cost reduction for a flight test is approximately a factor of 3 or 4 while the time is reduced by a minimum of two work weeks and a normal time period of one full working month.

b. Diagnoses of Problems and Techniques for Application

Up to this time, research has been performed in theoretical and experimental investigations of physical phenomena and processes in the Earth's atmosphere associated with the development of an experimental means of remotely measuring concentrations of gaseous constituents of the atmosphere.

(1) In view of the fact it is not currently possible to simulate accurately in the laboratory the infrared activity of the Earth and its dynamic atmosphere, theoretical techniques, such as line-by-line radiative transfer computer programs, must be applied to relate the voltage output of passive remote sensors to the total vertical gas burden measured. Extensive investigations and applications of existing programs were enacted in efforts to extract intelligence from raw flight test data obtained in June 1975. Weaknesses in the data reduction procedures were defined and investigated resulting in the implementation of a new data analysis procedure which will increase the time efficiency and reliability of data obtained in future test flights over homogeneous terrains.

Currently more efficient and flexible radiative transfer software is being developed for compatibility with remote sensor data reduction procedures.

(2) In the diagnosis of problems and techniques associated with the final application of the sensor, two more or less apparent major problems were addressed. These were:

- (a) The inherent ambiguity in the level-by-level constituent concentrations and temperatures for vertically integrated radiance measures provided by the sensor.
- (b) The development of analytic techniques for minimizing the noise-to-signal ratios in the data created by emissions from the Earth and more dense atmospheric constituents.
- (c) The results from the above would also be used to help guide subsequent instrument design and modification as well as help define the upper and lower limits (in both preferred periods and physical areas) for meaningful application of the sensor.

3. PROPOSED FOLLOW-ON RESEARCH

a. Evaluation of Sensor

In the coming months more statistical studies will be done on other types of sampling vessels: inflatable bags and stainless steel bottles other than our own so that a direct comparison of the various containers may be made.

Within the next few months a calibration system must also be developed since commercially available compressed gases normally used for gas chromatograph calibration have proved unreliable at the very low concentrations in which we are interested. A dynamic flow system is under consideration where the gases are continuously flowing and dynamically mixed to produce the desired concentration.

The problem of measuring SO_2 and NH_3 at the ambient clean air level will also be investigated, as ground truth measurements will be necessary for these contaminants during the coming year also. A study will be made of the various methods currently available for detection and measurement of these trace gases and a system will be developed for the taking of ground truth data for these gases.

b. Diagnosis of Problems and Application Techniques

(1) Laboratory experiments will be outlined for the purpose of verifying instrument software and refining input parameters and algorithms. An extension of research relating to the measurement of atmospheric constituents by means of passive remote sensors carried aboard aircraft or spacecraft will be undertaken. Continuation and extension of assistance in supplying meteorological and radiative transfer information for the purpose of specifying the required instrument performance characteristics and developing the computer programs which are required for reduction and interpretation of raw data produced by these sensors for both homogeneous and non-homogeneous terrains will be pursued. Assistance in defining new applications for the measurement techniques, locally and worldwide, will be supplied. Assistance and participation in planning

and executing flight experiments which will be designed to evaluate the sensors, the data reduction techniques, and the suitability of these techniques for the intended applications will be rendered.

The vertical ambiguity of concentrations and temperatures will have to be resolved for final application in the overall concept objectives. Several avenues were explored, each which would be applicable to a characteristic natural condition. The greatest progress was made for conditions simulating a surface-emitted gas during the night hours. Here, it assumed that the vertical wind and temperature profile were known within present meteorological accuracy. In this environment, the vertical distribution of a conservative surface-emitted substance is determinable from the wind and temperature field in terms of surface and upper level boundary values. By selecting an upper level where concentration is small and combining the atmospheric diffusion equation with the radiative transfer equation, the temperature sensitivities of the two equations are combined to form an equation in which an expression for the surface boundary concentration is defined in terms of the sensor radiance values and the presumed atmospheric wind and temperature distributions. This value may then be used as a boundary condition in the atmospheric diffusion equation to obtain concentration on a level-by-level basis. The solution requires a numerical integration by a successive approximation approach.

A numerical model for combining the two equations and integration for final solution has been completed and tested showing reasonable results, particularly with respect to the contribution of errors in the surface temperature and errors in assumed upper boundary values to overall noise levels. These show the critical need for noise suppression systems such as envisioned within the "filtered" sensor system discussed previously. The model is presently being adapted to simulate the NASA LaRC-designed "filtered" sensors.

An analytic formulation has been developed that shows promise for eliminating the very cumbersome spectral integrations in the solution of the above equation as applied to this specific problem.

(2) The technique for obtaining stratified concentration values from sensor radiance values will be adapted to the filtered sensor and tested to quantitatively assess the effectiveness of the filter.

A mathematical formulation that would permit the elimination of the cumbersome line-by-line spectral integration in data processing will be programmed and tested against actual laboratory and computer experiments. A most valuable potential of this technique will be a computer-time economical means of examining many spectral bands and instrument performance for optimum combinations and hopefully will be a big help in downstream system design and modification. This formulation is obtained by expressing absorption coefficients over a spectral band in terms of the mean and the deviation from the mean. By taking advantage of the fact that the total absorption by these trace gases over a band is a small quantity, the resulting integration over the spectral range is reduced to an expression involving the mean, the standard deviation, and the correlation coefficients between the absorption coefficients of different gases absorbing in the band. The extensive computer time required by the NASA radiative transfer model makes it very expensive to apply the model to a large number of spectral bands and atmospheric conditions.

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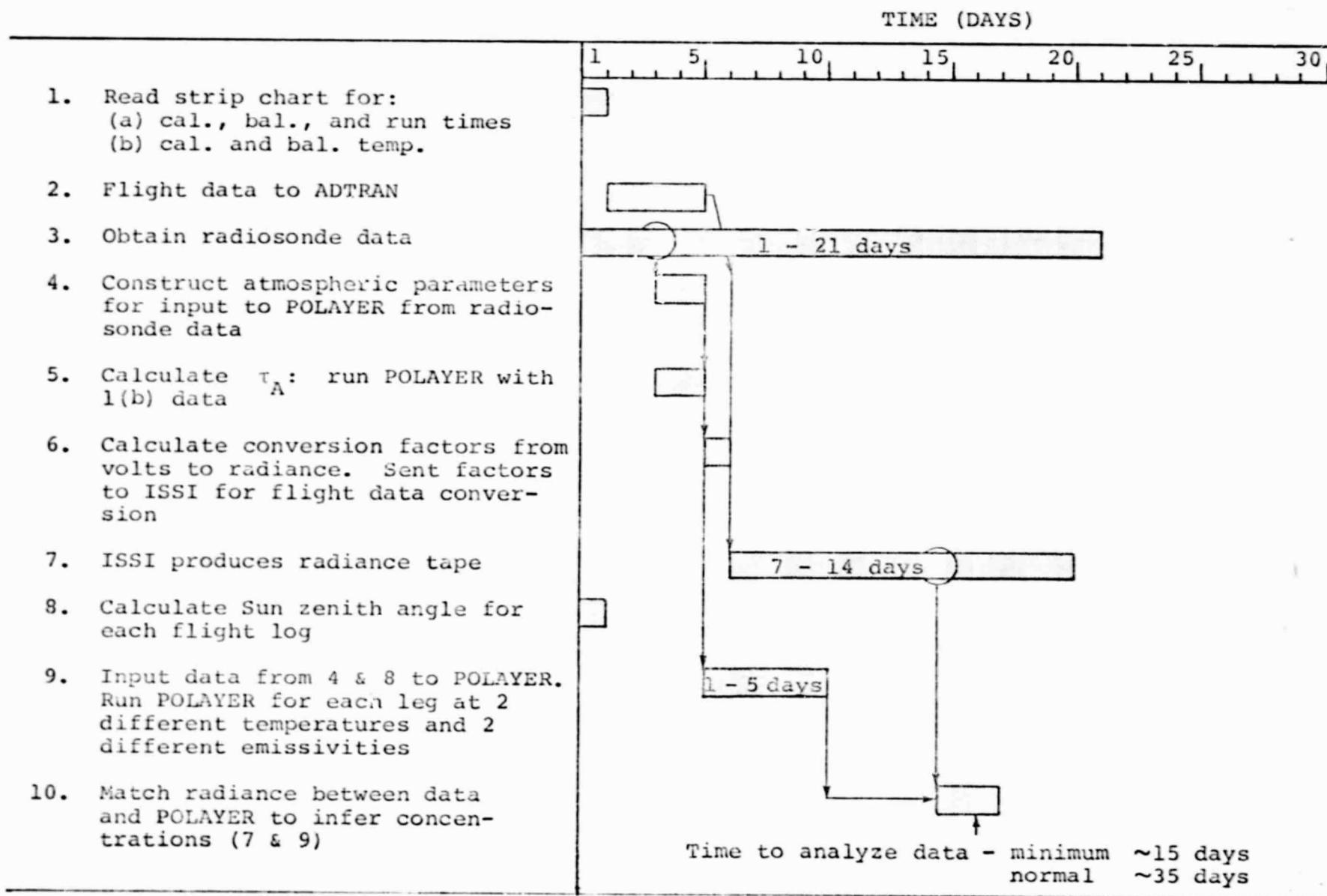
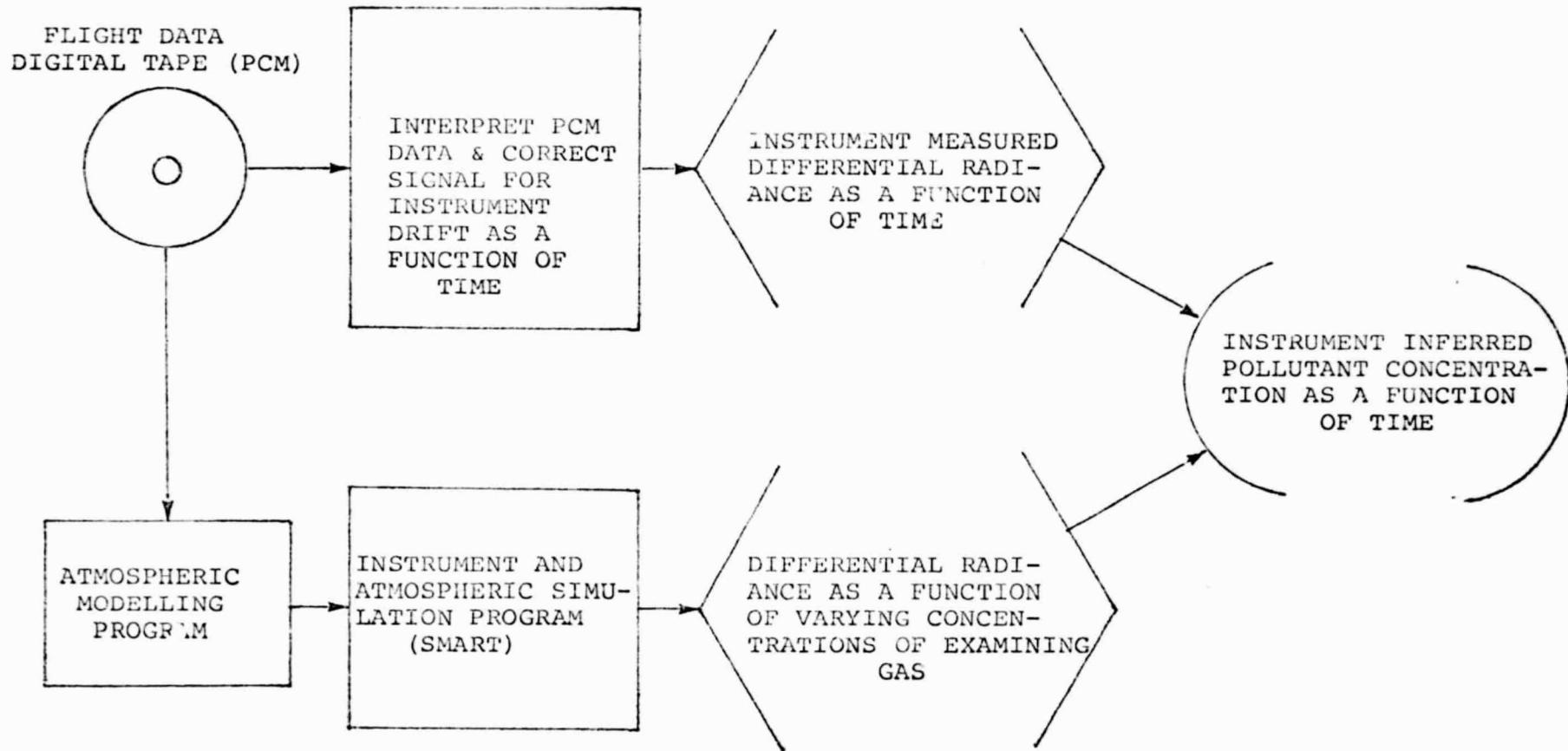


Figure 1. Current data analysis procedures.



Estimated time to analyze data: 3 to 6 days

Estimated cost: 15 computer runs - \$500

Figure 2. Proposed data analysis procedure.